

WKB formalism and a lower limit for the energy eigenstates of bound states for some potentials

Luis F. Barragán-Gil* and Abel Camacho†

*Departamento de Física, Universidad Autónoma Metropolitana-Iztapalapa
Apartado Postal 55-534, C.P. 09340, México, D.F., México.*

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In the present work the conditions appearing in the so-called WKB approximation formalism of quantum mechanics are analyzed. It is shown that, in general, a careful definition of an approximation method requires the introduction of two length parameters, one of them always considered in the text books on quantum mechanics, whereas the second one is usually neglected. Afterwards we define a particular family of potentials and prove, resorting to the aforementioned length parameters, that we may find an energy which is a lower bound to the ground energy of the system. The idea is applied to the case of a harmonic oscillator and also to a particle freely falling in a homogeneous gravitational field, and in both cases the consistency of our method is corroborated. This approach, together with the so-called Rayleigh–Ritz formalism, allows us to define an energy interval in which the ground energy of any potential, belonging to our family, must lie.

I. INTRODUCTION

In quantum mechanics the situation is, in a certain sense, quite similar to the situation in classical mechanics, namely, the number of physical systems of interest for which the corresponding motion equations can be solved exactly is not very large. Therefore approximation methods have been developed and play an important role in quantum mechanics. Among these approaches we may mention the WKB, Rayleigh–Ritz, or perturbation methods [1]. These different ideas have realms of applicability that not always intersect. For instance, WKB is applicable to states of the corresponding system characterized by very large values of a certain quantum number [2], and the variational method, also known as Rayleigh–Ritz, is employed to find bounds to the ground state energy of a quantum system [2].

In the present paper we will focus on the WKB method and analyze the conditions that appear in the implementation of it. It will be shown that, in general, they involve two conditions. Usually only one is considered, the remaining one is somehow neglected. Indeed, in all text books on quantum mechanics the fact that the method yields a good approximation only for the case in which there are several wavelengths between the corresponding classical turning points is very carefully explained, and mathematically implemented [2].

Nevertheless, there is an additional approximation that is always done, and implicitly introduced, namely, at a point on the potential curve a Taylor expansion for the potential is done, and then only a finite number of terms of this expansion are considered (usually two terms [1, 2]). Then this approximate Schrödinger equation is solved, and with it an auxiliary function is defined. This auxiliary function is employed to find the relation between the coefficients of the two involved WKB functions, one function on the left-hand side and a second one on the right-hand side of the classical turning point.

It has to be underlined that when this is done, in order to implement the method the solution (stemming from the approximate Schrödinger equation) is compared against the WKB wavefunction. This procedure is carried out on both sides of the corresponding classical turning point. We must distinguish, in connection with the approximate Schrödinger equation and its corresponding solution, that the validity region of the approximate equation (remember that it is obtained truncating the Taylor expansion for the potential) does define the region in which the corresponding solution can be applied. Of course, the solution to the approximate Schrödinger equation may have a definition domain larger than the region in which the approximate potential is valid, but if we use the solution at points outside the validity region of the approximate Schrödinger equation, then we use the solution to a potential that does not represent very good the physical situation. In other words, a rigorous procedure implies that the solution to the approximate Schrödinger equation has to be compared against the WKB wavefunction within the validity region of the aforementioned differential equation.

*Electronic address: brgl@xanum.uam.mx

†Electronic address: acq@xanum.uam.mx

This last remark implies that there are two different length parameters involved in the WKB procedure: (i) the first one tells us that we cannot be very close to the classical turning point, otherwise the approximate wavefunction diverges [1, 2]; (ii) the second length parameter appears when we recognize that the comparison between the solution to the approximate Schrödinger equation and the WKB wavefunction has to be carried out within the validity region of the approximate Schrödinger equation. Usually, only the first length parameter is considered in the text books on quantum mechanics [1, 2], the second one is always neglected, and we may wonder if a careful analysis of it is necessary, since we seek an approximate solution, valid at both sides of our classical turning points.

In the present work we will take into account both conditions and show that a careful analysis of them leads us to some interesting facts. For instance, we will show that it is possible to find a lower bound to the ground energy of the so-called bound states for some potentials. This is an interesting result, since the current approximation methods cannot render a lower bound to the ground state, only the Rayleigh–Ritz method provides a formalism which allows us to obtain, via an energy functional, an energy which cannot be smaller than ground energy of the corresponding system. With our method the ground energy is always larger than the energy that our method provides. Clearly, joining the conclusions of Rayleigh–Ritz with ours we may find an interval in which the ground energy of a one-dimensional system has to lie. Though the present approach is restricted to a certain family of potentials we will prove that the case of a harmonic oscillator, or a particle freely falling in a homogeneous gravitational field, among other potentials, belong to this family.

II. VALIDITY REGION FOR THE WKB FORMALISM

The core point in the WKB formalism is related to the fact that the coefficients appearing in the different regions, which are separated by the corresponding classical turning points, are matched resorting to the so-called connection formulas [1]. These formulas are obtained introducing an approximate Schrödinger equation at the classical turning point, solving it, finding its asymptotic behavior, and comparing the coefficients against those stemming from the WKB formalism. The phrase *an approximate Schrödinger equation at the classical turning point* plays here a very relevant role, and has to be explained in a very clear manner.

Let us now proceed to do this. Consider now one of the classical turning points, say x_0 . A Taylor expansion at this point, for the potential is introduced ($V : I \rightarrow \mathbb{R}$, where $I \subseteq \mathbb{R}$)

$$V(x) = V(x_0) + V'(x_0)(x - x_0) + \frac{V''(x_0)}{2!}(x - x_0)^2 + \dots \quad (1)$$

The approximate time-independent Schrödinger equation is defined resorting to the first non-vanishing derivative at x_0 , usually the first-order derivative

$$-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} + \left[V(x_0) + V'(x_0)(x - x_0) \right] \psi(x) = E\psi(x). \quad (2)$$

The solutions to (2) are Airy functions [1]. The second step is to take the asymptotic form for the corresponding solutions to (2). This has to be done because the main idea is to use this approximate equation as a patching expression, and employ it to connect the expressions stemming from the WKB formalism on both sides of each one of the classical turning points. Here the verb *connect* means to find the relations between the coefficients of the solutions obtained with WKB on both sides of the classical turning point. Since this part of the method requires the WKB wavefunctions, then the comparison between the Airy functions and the WKB wavefunctions has to be done in a region where the latter are well defined, i.e., sufficiently far from the classical turning point [1].

Up to this point everything is quite clear in the textbooks on quantum mechanics. Nevertheless, there is an issue which is not addressed, and is a relevant one. Namely, the comparison has to be carried out far enough from the classical turning point, but resorting to the asymptotic behavior of the Airy functions this last argument is not enough. Indeed, we must be sure that in the region where the comparison is done the approximation chosen for the Schrödinger equation is a good one, otherwise we would be employing the asymptotic behavior of the solutions of an equation which is not a good approximation in the region where the comparison is done. In other words, a careful procedure should check that the region in which WKB wavefunctions are valid contains as a subset an interval in which (2) is valid, i.e., we do not need to take into account the second order derivative, for instance.

This last statement can be rephrased asserting that the region of the comparison is defined as follows (here from the very beginning we assume the usual case, a linear approximation for the Schrödinger equation, additionally recall that at the classical turning point $E = V(x_0)$)

$$V(x) \approx E + V'(x_0)(x - x_0). \quad (3)$$

If this last approximation is a good one, then the terms of the form $(x - x_0)^k$, with $k \geq 2$, can be neglected and this assertion implies

$$|V'(x_0)(x - x_0)| > |\frac{V''(x_0)}{2!}(x - x_0)^2|. \quad (4)$$

This last expression defines the validity region of (2). Indeed, (4) entails that

$$|2\frac{V'(x_0)}{V''(x_0)}| > |(x - x_0)|. \quad (5)$$

In other words, if the matching is done in a region which violates this last condition, then the approximate Schrödinger equation should consider higher-order derivatives. Notice that the condition is a function of the involved classical turning point, x_0 , in other words, the size of the validity region depends upon x_0 , it is not, in the general case, constant.

The use of the WKB method requires an additional condition [1], the one can be tracked down to the fact that the wavelength of the corresponding particle has to be much smaller than the region in which the potential has a noticeable change in its value

$$\frac{2|E - V(x)|}{|dV/dx|} \gg \lambda = \frac{\hbar}{\sqrt{2m[E - V(x)]}}. \quad (6)$$

Harking back to (1) we impose the condition that

$$\limsup |\frac{V^{(l+1)}(x_0)}{V^{(l)}(x_0)}(x - x_0)| < 1. \quad (7)$$

This is tantamount to ask for the absolute convergence of the Taylor series of $V(x)$ [3]. Since this last expression is valid for all $x \in I$, then $\limsup |\frac{V^{(l+1)}(x_0)}{V^{(l)}(x_0)}| = 0$. This condition is not so stringent as it may seem, for instance, the potential of a harmonic oscillator satisfies it, i.e., $V^{(3)}(x) = 0, \quad \forall x \in \mathbb{R}$.

III. VALIDITY REGIONS OF THE SEMICLASSICAL APPROXIMATION

Let us now proceed to define the family of potentials which will be addressed in the present work.

Firstly, if $x \leq 0$, the potential becomes infinite. Secondly, it is a monotonically increasing function and

$$\lim_{x \rightarrow 0^+} V(x) \rightarrow 0, \quad \text{as } x \rightarrow 0^+ \quad (8)$$

Additionally, it possesses bound states, in such a way that the corresponding energy eigenvalues are $\{E_0, E_1, \dots\}$, where $E_l < E_n$, if $l < n$.

Let us now suppose that the first and second derivatives of the potential do not vanish $\forall x \in \mathbb{R}^+$. This condition is introduced in order to have in our family the case of a truncated harmonic oscillator. The case of a particle freely falling in a homogeneous gravitational field will also be addressed here, though for this potential the second derivative vanishes we may analyze it. The possibility of resorting to the WKB method, using a linear approximation for the potential energy at the classical turning point x_0 , is feasible at those points x such that they fulfill (5) and (6). These two conditions imply

$$\alpha^2 \left| \frac{V''(x_0)}{2} \frac{x_0 - x}{\alpha} \right| > \left[\sqrt{\frac{\hbar^2}{8m}} \alpha \frac{V''(x_0)}{2} \right]^{2/3} \left| 1 - \frac{4}{3} \frac{x_0 - x}{\alpha} \right|. \quad (9)$$

Here we have defined the length parameter

$$\alpha = 2|V'(x_0)/V''(x_0)|. \quad (10)$$

This assertion may be rephrased stating that WKB can not be applied at a point x in the classical region (the one is defined by the interval $J = (0, x_0]$) if the following inequality holds

$$\alpha^2 \left| \frac{V''(x_0)}{2} \frac{x_0 - x}{\alpha} \right| \leq \left[\sqrt{\frac{\hbar^2}{8m}} \alpha \frac{V''(x_0)}{2} \right]^{2/3} \left| 1 - \frac{4}{3} \frac{x_0 - x}{\alpha} \right|. \quad (11)$$

If the use of a linear approximation to the potential is inconsistent we could try to employ the WKB formalism considering higher-order derivatives in the approximate Schrödinger equation, and we would end up with an inequality (though a more complicated one) and a new length parameter, the one would be given by the expression $\alpha = (l+1)|V^{(l)}(x_0)/V^{(l+1)}(x_0)|$.

Let us now analyze the implications of the breakdown of the linear approximation, and study its consequences, if any, upon the energy eigenvalues.

Defining

$$\gamma = \left\{ \frac{\hbar^2}{4m\alpha^4 V''(x_0)} \right\}^{1/3}, \quad (12)$$

$$z = \frac{x_0 - x}{\alpha}. \quad (13)$$

We may cast (11) as follows

$$|z| \leq \gamma |1 - 4z/3|. \quad (14)$$

We consider now the classical region J , and restrict x to it, then $z \in [0, x_0/\alpha]$.

This last condition allows us to define the following two functions

$$f : [0, x_0/\alpha] \rightarrow \mathbb{R}, \quad (15)$$

$$g : [0, x_0/\alpha] \rightarrow \mathbb{R}, \quad (16)$$

$$f(z) = z, \quad (17)$$

$$g(z) = \gamma |1 - 4z/3|. \quad (18)$$

It is readily seen that $\forall z \in [0, x_0/\alpha]$ we have that $f(z) \geq 0$. On the other hand, our function $g(z)$ may change sign in this interval. Indeed,

$$\gamma |1 - 4z/3| = \begin{cases} \gamma [1 - 4z/3], & \text{when } z \leq 3/4 \\ \gamma [-1 + 4z/3], & \text{when } z \geq 3/4 \end{cases} \quad (19)$$

We have two possibilities

A. First Case ($x_0/\alpha \leq 3/4$)

Then the condition that implies the breakdown of WKB reads

$$z \leq \gamma[1 - 4z/3]. \quad (20)$$

The border that divides the regions, in which WKB is valid from the one in which it is not valid, is given by

$$z = \gamma[1 - 4z/3], \quad (21)$$

$$z = \frac{\gamma}{1 + 4\gamma/3}. \quad (22)$$

In other words, in the region $z \in [0, \frac{\gamma}{1+4\gamma/3}]$ WKB cannot be used, and in $z \in [\frac{\gamma}{1+4\gamma/3}, x_0/\alpha]$ WKB is valid.

Notice that if the interval $z \in [\frac{\gamma}{1+4\gamma/3}, x_0/\alpha]$ becomes one point, then in the region $x \in (0, x_0]$ WKB cannot be used. This happens when

$$\frac{\gamma}{1 + 4\gamma/3} = x_0/\alpha, \quad (23)$$

This condition can be cast as follows

$$\frac{\hbar^2}{8m} = \frac{\alpha x_0^3}{2} V''(x_0) \left[1 - \frac{4x_0}{3\alpha}\right]^{-3}. \quad (24)$$

The roughest approximation allow us to rewrite (24) as

$$\frac{\hbar^2}{8m} = x_0^3 V'(x_0). \quad (25)$$

Additionally, we have the condition $x_0/\alpha \leq 3/4$, which implies

$$x_0 \leq \frac{3V'(x_0)}{2V''(x_0)}. \quad (26)$$

Consider now the following potential ($\beta > 0$)

$$V(x) = \begin{cases} \beta x^n, & \text{when } x > 0 \\ \infty, & \text{when } x \leq 0 \end{cases}. \quad (27)$$

(26) implies that for this kind of potentials

$$n \leq 5/2. \quad (28)$$

Notice that the fulfillment of (26) for the aforementioned family of potentials does not involve the value of β , only of n . Under this condition we may find some important potentials of quantum physics, namely, the harmonic oscillator ($n = 2$) and a particle freely falling in a homogeneous gravitational field ($n = 1$).

The value of x_0 , using (25) and (27), is given by

$$x_0 = \left(\frac{\hbar^2}{8\beta m n} \right)^{1/(n+2)}. \quad (29)$$

From this last expression, additionally, we find the following energy

$$E_{cl}^{(1)} = \beta x_0^n = \frac{\hbar^2}{8mnx_0^2}. \quad (30)$$

The meaning of this energy is the following one. For this kind of potential this is the minimum energy that a particle can have in order to, with a linear approximation to the potential, be able to employ WKB. Indeed, notice that x_0 is the smallest value of the coordinate at which the aforementioned formalism can be employed, and since we have assumed, from the very beginning, a monotonically increasing potential, then we deduce that if a particle has an energy smaller than (30), then WKB cannot be employed.

At this point we may wonder if this energy has some physical meaning. We will show that it is a lower bound to the eigenenergies of the corresponding bound states, i.e., all the eigenenergies stemming from the solution to the corresponding Schrödinger equation, and related to bound states, are larger or equal to $E_{cl}^{(1)}$. This assertion will be proved in section IV.

B. Second Case ($x_0/\alpha \geq 3/4$)

In this case the breakdown of WKB involves expression (19), and clearly the first point of interest is related to the fulfillment of expression (21). In other words, once again, in the region $z \in [0, \frac{\gamma}{1+4\gamma/3}]$ WKB cannot be used. But, since we have that $x_0/\alpha \geq 3/4$, now the breakdown of WKB can include a new interval, the one is absent when $x_0/\alpha \leq 3/4$. Indeed, consider now the possibility in which

$$z = \gamma[-1 + 4z/3]. \quad (31)$$

This happens when

$$z = \frac{\gamma}{-1 + 4\gamma/3}. \quad (32)$$

Clearly, the case $4\gamma/3 = 1$ has to be discarded in this last equation. Nevertheless, we must also analyze the case in which $4\gamma/3 = 1$. Expression (20) tells us that in the region $z \in [\frac{\gamma}{1+4\gamma/3}, x_0/\alpha]$ WKB can be used, this is when $4\gamma/3 = 1$. This is easy to understand since the slope of the two straight lines, $f(z) = z$ and $g(z) = \gamma[-1 + 4z/3]$, is the same, $4\gamma/3 = 1$.

Harking back to the case $4\gamma/3 \neq 1$, we conclude that if $\frac{\gamma}{-1+4\gamma/3} \leq x_0/\alpha$, then we have three different regions, namely:

- (i) If $z \in [0, \frac{\gamma}{1+4\gamma/3}]$ WKB cannot be used; and it is related to the fact that we are too close to the classical turning point and in consequence (6) is not valid.
- (ii) If $z \in [\frac{\gamma}{1+4\gamma/3}, \frac{\gamma}{4\gamma/3-1}]$ WKB can be used;
- (iii) Finally, when $z \in [\frac{\gamma}{4\gamma/3-1}, x_0/\alpha]$ WKB loses, once again, its validity, but this time the breakdown of the method emerges because the approximation introduced for the Schrödinger equation at the classical turning point is violated, see expression (10).

Of course, this last possibility occurs only when

$$3/4 < \frac{\gamma}{4\gamma/3 - 1} \leq x_0/\alpha. \quad (33)$$

This last condition can be cast as follows

$$\frac{\hbar^2}{8m} \geq \left(3/4\right)^3 \alpha^4 \frac{V''(x_0)}{2}. \quad (34)$$

Consider now the case in which the potential is given by (27). One of our previous results, see (28), imposes as condition $n > 5/2$. Then we obtain as condition for the existence of the region defined by $z \in [\frac{\gamma}{4\gamma/3-1}, x_0/\alpha]$ the following inequality

$$\frac{\hbar^2}{8mx_0^2} \geq \left(\frac{2}{3[n-1]}\right)^3 nV(x_0). \quad (35)$$

This last expression allows us to define the following energy

$$E_{cl}^{(1)} = \left(\frac{3[n-1]}{2}\right)^3 \frac{\hbar^2}{8mnx_0^2}. \quad (36)$$

C. Comparison between the two cases

If $x_0/\alpha \geq 3/4$, then we cannot obtain the value of n without knowing also the value of β (the one appears in $V(x_0)$), as expression (35) clearly shows. This does not happen in the first situation ($x_0/\alpha \leq 3/4$), see expression (28), in which the condition upon n is independent from the value of β , though x_0 does involve β , see (29).

An additional difference between these two cases lies in the fact that if ($x_0/\alpha \leq 3/4$) then we may find a family of potentials such that the analysis contains only one region, see expression (24), in which WKB is not valid (in the interval $(0, x_0)$ the conditions imposed by WKB cannot be satisfied), whereas in the other situation the analysis shows the possibility of having two or three regions, and in one of them WKB can always be employed.

As a byproduct we have obtained for the first case an energy, see expression (30) such that for energies smaller than it the WKB method cannot be used. Similarly, for the second situation, expression (36) defines an energy such that if the energy of our particle is smaller than that provided by (36), then WKB cannot be used. In other words, in both cases we find a lower bound for the validity of the method, the one includes a linear approximation for the Schrödinger equation at the classical turning point.

IV. LOWER BOUND FOR THE GROUND STATE ENERGY

Let us now consider the classical energy $E_{cl}^{(1)} = V(x_0)$ obtained previously, see expressions (30) and (36). The meaning of this energy is the following one. For the kind of potential under consideration this is the minimum energy that a particle can have in order to, with a linear approximation to the potential, be able to employ WKB. Indeed, notice that x_0 is the smallest value of the coordinate at which the aforementioned formalism can be employed, and since we have assumed, from the very beginning, a monotonically increasing potential, then we deduce that if a particle has an energy smaller than (30) or (36), then this energy can not be obtained via WKB.

At this point we may wonder if this energy has some physical meaning. Let us now answer this question. We will conjecture that if

$$E_{cl}^{(1)} \leq \frac{\hbar^2}{8mx_0^2}, \quad (37)$$

then it is a lower bound to the eigenenergies of the corresponding bound states, i.e., all the eigenenergies stemming from the solution to the corresponding Schrödinger equation, and related to bound states, are larger or equal to $E_{cl}^{(1)}$.

Let us now consider the lower energy eigenstates of a quantum system subject to a potential satisfying our requirements. Under this condition WKB may be used, though it provides energies that are not a good approximation to the correct ones. We now proceed to prove that when $E_{cl}^{(1)}$ satisfies (37), then it does define a lower bound to the ground energy of the system. Consider the energy E_0 of the ground state and assume that it intersects the potential at x_g , i.e., $E_0 = V(x_g)$. Here we have two possibilities:

(i) x_g lies on the right-hand side of x_0 . In this case E_0 can be obtained via WKB, and since $E_{cl}^{(1)}$ is the smallest energy that allows the use of this approach, then $E_{cl}^{(1)} \leq E_0$, and we are done;

(ii) Consider the remaining possibility, $x_g < x_0$. Since we have assumed a monotonically increasing potential, then this last condition implies that $V(x_g) < V(x_0)$.

The idea here is to proceed by contradiction, namely, assume that $x_g < x_0$, a fact that implies $V(x_g) < V(x_0)$, and resorting to the fundamentals of quantum mechanics we will show that this assumption leads to an inconsistency for those potentials fulfilling (37).

According to quantum mechanics the distance that the wave function (of a bound state) tunnels inside the classically forbidden region becomes larger as the energy grows. Indeed, in the aforementioned region the wavefunction behaves as $\psi(x) \approx \exp\left\{-\frac{1}{\hbar} \int_a^x \sqrt{2m[V(z) - E]} dz\right\}$ [4].

Let us now recall the uncertainty relation

$$\Delta x \Delta p \geq \frac{\hbar}{2}. \quad (38)$$

For the ground state the tunnelling distance is the smallest one, and if x_g denotes the intersection of the ground energy with potential, then $(0, x_g]$ is the classical region, and we may state that

$$\Delta x \sim x_g. \quad (39)$$

This last expression says that the probability of finding the particle in the classically forbidden region is almost zero, and in consequence, the uncertainty region associated to the position of the particle is related to the classical region, in which the wavefunction has an oscillatory behavior. Bearing this in mind the uncertainty relation can be cast in the following form

$$x_g \sqrt{2m[E_0 - \langle V \rangle - (\langle p \rangle)^2]} \geq \frac{\hbar}{2}. \quad (40)$$

Where the averages are calculated with the wavefunction of the ground state. Since we have assumed that $V(x) \geq 0$, $\forall x \in \mathbb{R}^+$, then (40) implies

$$x_g \sqrt{2mE_0} \geq \frac{\hbar}{2}. \quad (41)$$

Then the ground state energy satisfies the condition

$$E_0 \geq \frac{\hbar^2}{8mx_g^2}. \quad (42)$$

And since our initial hypothesis has been the condition $x_g < x_0$, then

$$\frac{\hbar^2}{8mx_0^2} \leq \frac{\hbar^2}{8mx_g^2}. \quad (43)$$

Nevertheless, we have assumed from square one the validity of (37), and hence we find a contradiction. Indeed, our three initial conditions (expression (37) and $x_g < x_0$ and the uncertainty relation) imply $E_{cl}^{(1)} \leq E_0$. Nevertheless, since the potential has been assumed monotonically increasing, then $x_g < x_0 \Rightarrow V(x_g) < V(x_0)$, and in consequence, we find that the simultaneous use of these three conditions is, logically, inconsistent, and therefore the case $x_g < x_0$ has to be discarded, if expression (37) and the uncertainty relation are to be kept. Clearly, we conclude that $E_{cl}^{(1)}$ provides a lower bound for the ground energy. We now proceed to analyze if any of our two possible cases satisfies (37).

A. First case

Consider now a potential given by (27), with $1 \leq n \leq 5/2$. Then, $E_{cl}^{(1)} = \frac{\hbar^2}{8mnx_0^2}$, and condition (37) is fulfilled.

In other words, if $1 \leq n \leq 5/2$, then $E_{cl}^{(1)}$ does provide a lower bound to the ground energy of the corresponding system.

B. Second case

The remaining possibility, $n > 5/2$, cannot be analyzed in the context of our approach. Indeed, notice that now we require the fulfillment of the following condition

$$\frac{\hbar^2}{8mx_0^2} \geq \left(\frac{3[n-1]}{2}\right)^3 \frac{\hbar^2}{8mnx_0^2}. \quad (44)$$

This last condition can be cast as

$$\left(\frac{3}{2}\right)^3 \leq \frac{n}{(n-1)^3}. \quad (45)$$

Clearly, not only (45) has to be satisfied, additionally $n > 5/2$. A fleeting glimpse shows that this is impossible, in other words, we cannot use the present approach to find a lower bound for potential of the form $V(x) = \beta x^n$, if $n > 5/2$.

V. SOME PARTICULAR POTENTIALS

Notice that under the condition $n \leq 5/2$ we may find the potential associated to a harmonic oscillator, or a particle freely falling in a homogeneous gravitational field. We know proceed to calculate the bounds for these two potentials that our method provides. We use these two cases to corroborated our predictions, since we need potentials whose exact eigenenergies are already known.

A. Harmonic Oscillator

A particular case of the situation just mentioned is the potential associated to a harmonic oscillator. Notice that for this case the condition $n < 5/2$ is fulfilled, and in consequence, if our argument is valid, then we expect to obtain a lower bound to the ground energy.

$$V(x) = \begin{cases} \frac{m}{2}\omega^2 x^2, & \text{when } x > 0 \\ \infty, & \text{when } x < 0 \end{cases}. \quad (46)$$

In this case (see expression (29))

$$x_0 = \left(\frac{1}{8}\right)^{1/4} \lambda_0, \quad (47)$$

$$\lambda_0 = \sqrt{\frac{\hbar}{m\omega}}, \quad (48)$$

$$E_{cl}^{(1)} = \frac{1}{2\sqrt{8}}\hbar\omega \quad (49)$$

The eigenenergies of a harmonic oscillator read $E_n = \hbar\omega[(2n+1) + 1/2]$, in this case n is an integer. Clearly, since we have the truncated harmonic oscillator potential, only the odd wave functions are allowed and, in consequence, the ground state is given by $E_0 = \frac{3}{2}\hbar\omega$. Here we have that, indeed, $E_{cl}^{(1)} < E_0$.

B. Free Fall

Another interesting situation in quantum mechanics, the one has exact solution, is the case of a particle falling in a homogeneous gravitational field [5]. Here the potential satisfies the condition

$$V(x) = \begin{cases} mgx, & \text{when } x > 0 \\ \infty, & \text{when } x \leq 0 \end{cases}. \quad (50)$$

The eigenenergies are given by ($n \in \mathbb{N}$)

$$E_n = \frac{\hbar^2}{2ml^2} \left\{ \frac{3\pi}{4} \left[2n - \frac{1}{2} \right] \right\}^{2/3}, \quad (51)$$

$$\frac{1}{l^3} = \frac{2m^2g}{\hbar^2}. \quad (52)$$

For this type of potential the second derivative vanishes in the region $(0, \infty)$, and hence, the condition that determines the minimum distance x_0 is given by

$$x_0 \leq \frac{1}{2} \left(\frac{\hbar^2}{m^2g} \right)^{1/3}. \quad (53)$$

Since the potential is linear, then, clearly, the linear approximation to Schrödinger equation is always valid, and the breakdown of the method is only related to the violation of (6).

The ensuing energy reads

$$E_{cl}^{(1)} = \frac{\hbar^2}{\sqrt[3]{32} ml^2}. \quad (54)$$

Notice that the energy eigenvalues can be cast as follows

$$E_n = E_{cl}^{(1)} \left\{ \frac{3\pi}{2} \left[2n - \frac{1}{2} \right] \right\}^{2/3}. \quad (55)$$

The ground state corresponds to $n = 0$, and then (55) becomes

$$E_0 = E_{cl}^{(1)} \left\{ -\frac{3\pi}{4} \right\}^{2/3}. \quad (56)$$

Clearly, once again, the condition, $E_0 > E_{cl}^{(1)}$ is fulfilled, $\left\{ -\frac{3\pi}{4} \right\}^{2/3} > 1$.

VI. CONCLUSIONS

In the present work it has been shown that the so-called WKB approximation method involves two length parameters which have to be introduced in the calculation of the relevant variables. Usually, only one of these length parameters is considered in the text books on quantum mechanics [1, 2], the second one is always neglected. These parameters are related to different conditions that have to be fulfilled in order to have a mathematically consistent approximation method: (i) the first one tells us that we cannot be very close to the classical turning point, otherwise the approximate wavefunction diverges [1, 2], see expression (6); (ii) whereas the second length parameter appears when we recognize that the comparison between the solution to the approximate Schrödinger equation and the WKB wavefunction has to be carried out within the validity region of the aforementioned motion equation, see expression (5).

Both conditions have been taken into account and it has been shown that a careful analysis of them leads us to some interesting facts. For instance, it is possible to find a lower bound to the ground energy for some potentials, i.e., those whose behavior goes like $V(x) = \beta x^n$, $\beta > 0$ and $1 \leq n \leq 5/2$. Joining the present conclusions with the so-called Rayleigh–Ritz method allows us to find an interval in which the ground energy of a one-dimensional system has to lie. Additionally, some examples of the approach have been explicitly calculated, for instance, the case of a harmonic oscillator, or a particle freely falling in a homogeneous gravitational field, and it has been shown that the energy deduced with our arguments is, indeed, smaller than the ground energy of the corresponding system.

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